Succinic acid, hept-2-yl 1-cyclopentylethyl ester

Inchi: InChI=1S/C18H32O4/c1-4-5-6-9-14(2)21-17(19)12-13-18(20)22-15(3)16-10-7-8-11-16/h1

InchiKey: JAFGWHZDHQGLDS-UHFFFAOYSA-N

Formula: C18H32O4

SMILES: CCCCCC(C)OC(=O)CCC(=O)OC(C)C1CCCC1

Mol. weight [g/mol]: 312.44

Physical Properties

Property code	Value	Unit	Source
gf	-335.49	kJ/mol	Joback Method
hf	-854.53	kJ/mol	Joback Method
hfus	34.84	kJ/mol	Joback Method
hvap	73.45	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	4.401		Crippen Method
mcvol	268.500	ml/mol	McGowan Method
pc	1415.44	kPa	Joback Method
rinpol	2105.00		NIST Webbook
rinpol	2105.00		NIST Webbook
tb	778.22	K	Joback Method
tc	973.59	K	Joback Method
tf	417.84	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	842.98	J/mol×K	778.22	Joback Method
cpg	861.60	J/mol×K	810.78	Joback Method
cpg	879.06	J/mol×K	843.34	Joback Method
cpg	895.36	J/mol×K	875.91	Joback Method
cpg	910.54	J/mol×K	908.47	Joback Method
cpg	924.61	J/mol×K	941.03	Joback Method
cpg	937.61	J/mol×K	973.59	Joback Method
dvisc	0.0018040	Pa×s	417.84	Joback Method

dvisc	0.0007940	Pa×s	477.90	Joback Method
dvisc	0.0004198	Pa×s	537.97	Joback Method
dvisc	0.0002522	Pa×s	598.03	Joback Method
dvisc	0.0001663	Pa×s	658.09	Joback Method
dvisc	0.0001176	Pa×s	718.16	Joback Method
dvisc	0.0000877	Pa×s	778.22	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391412&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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